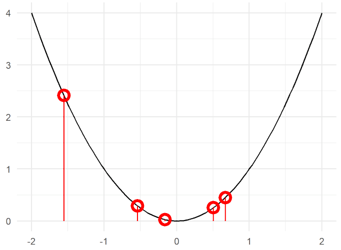
Introduction to Machine Learning

Regression Losses: L2-loss



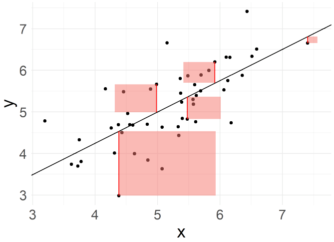
Learning goals

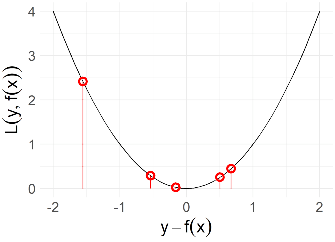
- Derive the risk minimizer of the L2-loss
- Derive the optimal constant model for the L2-loss

L2-LOSS

$$L(y, f(\mathbf{x})) = (y - f(\mathbf{x}))^2 \quad \text{or} \quad L(y, f(\mathbf{x})) = 0.5\,(y - f(\mathbf{x}))^2$$

- Tries to reduce large residuals (if residual is twice as large, loss is 4 times as large), hence outliers in y can become problematic
- Analytic properties: convex, differentiable (gradient no problem in loss minimization)
- Residuals = Pseudo-residuals: $\tilde{r} = -\frac{\partial 0.5(y - f(\mathbf{x}))^2}{\partial f(\mathbf{x})} = y - f(\mathbf{x}) = r$





L2-LOSS: RISK MINIMIZER

Let us consider the (true) risk for $\mathcal{Y} = \mathbb{R}$ and the *L*2-Loss $L(y, f(\mathbf{x})) = (y - f(\mathbf{x}))^2$ with unrestricted $\mathcal{H} = \{f : \mathcal{X} \to \mathbb{R}^g\}$.

- By the law of total expectation

$$
\begin{aligned}
\mathcal{R}_L(f) &= \mathbb{E}_{xy}\left[L(y, f(\mathbf{x}))\right] = \mathbb{E}_x\left[\mathbb{E}_{y|x}\left[L(y, f(\mathbf{x})) \mid \mathbf{x} = \mathbf{x}\right]\right] \\
&= \mathbb{E}_x\left[\mathbb{E}_{y|x}\left[(y - f(\mathbf{x}))^2 \mid \mathbf{x} = \mathbf{x}\right]\right].
\end{aligned}
$$

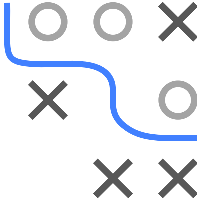
- Since $\mathcal{H}$ is unrestricted, at any point $\mathbf{x} = \mathbf{x}$, we can predict any value c we want. The best point-wise prediction is the cond. mean

$$
f^*(\mathbf{x}) = \text{argmin}_c \mathbb{E}_{y|x}\left[(y - c)^2 \mid \mathbf{x} = \mathbf{x}\right] \overset{(*)}{=} \mathbb{E}_{y|x}\left[y \mid \mathbf{x}\right].
$$

$^{(*)}$ follows from:

$$
\begin{aligned}
& \text{argmin}_c \mathbb{E}\left[(y - c)^2\right] = \text{argmin}_c \underbrace{\mathbb{E}\left[(y - c)^2\right] - (\mathbb{E}[y] - c)^2}_{=\text{Var}[y - c] = \text{Var}[y]} + (\mathbb{E}[y] - c)^2 \\
= \quad & \text{argmin}_c \text{Var}[y] + (\mathbb{E}[y] - c)^2 = \mathbb{E}[y].
\end{aligned}
$$

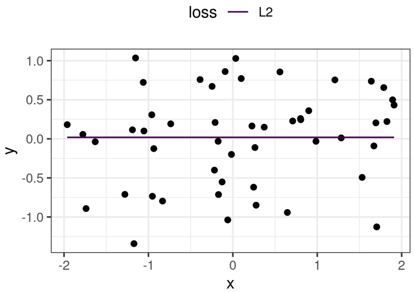
L2-LOSS: OPTIMAL CONSTANT MODEL



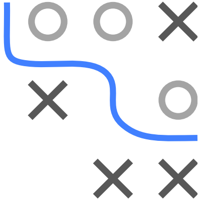
The optimal constant model in terms of the (theoretical) risk for the L2 loss is the expected value over y:

$$f(\mathbf{x}) \quad = \quad \mathbb{E}_{y \mid \mathbf{x}}\left[y \mid \mathbf{x}\right] \stackrel{\text{drop } \mathbf{x}}{=} \mathbb{E}_{y}\left[y\right]$$

The optimizer of the empirical risk is $\bar{y}$ (the empirical mean over $y^{(i)}$), which is the empirical estimate for $\mathbb{E}_{y}\left[y\right]$.



L2-LOSS: OPTIMAL CONSTANT MODEL / 2



Proof:

For the optimal constant model $f(\mathbf{x}) = \theta$ for the L2-loss $L(y, f(\mathbf{x})) = (y - f(\mathbf{x}))^2$ we solve the optimization problem

$$\arg\min_{f \in \mathcal{H}} \mathcal{R}_{\text{emp}}(f) = \arg\min_{\theta \in \mathbb{R}} \sum_{i=1}^{n} (y^{(i)} - \theta)^2.$$

We calculate the first derivative of $\mathcal{R}_{\text{emp}}$ w.r.t. θ and set it to 0:

$$\begin{aligned}
\frac{\partial \mathcal{R}_{\text{emp}}(\boldsymbol{\theta})}{\partial \theta} = -2 \sum_{i=1}^{n} \left(y^{(i)} - \theta\right) &\overset{!}{=} 0 \\
\sum_{i=1}^{n} y^{(i)} - n\theta &= 0 \\
\hat{\theta} &= \frac{1}{n} \sum_{i=1}^{n} y^{(i)} =: \bar{y}.
\end{aligned}$$

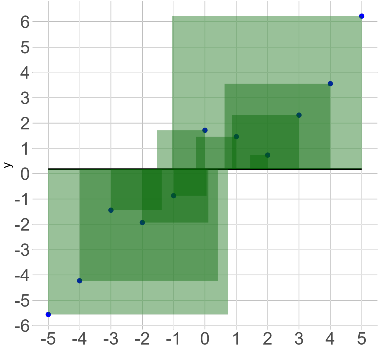
L2 LOSS MEANS MINIMIZING VARIANCE

Rethinking what we just did: We optimized for a constant whose squared distance to all data points is minimal (in sum, or on average). This turned out to be the mean.

What if we calculcate the loss of $\hat{\theta} = \bar{y}$? That's $\mathcal{R}_{\text{emp}} = \sum_{i=1}^{n}(y^{(i)} - \bar{y})^2$.

Average this by $\frac{1}{n}$ or $\frac{1}{n-1}$ to obtain variance.

Optimal constant model gives "unscaled" variance



- Generally, if model yields unbiased predictions, $\mathbb{E}_{y \mid \mathbf{x}}[y - f(\mathbf{x}) \mid \mathbf{x}] = 0$, using $L2$-loss means minimizing variance of model residuals
- Same holds for the pointwise construction / conditional distribution considered before